ANNEX II

Progress report on the project

“Development of the Technical and Policy Frameworks for Transboundary Air Pollution Assessment and Abatement of North-East Asia”

Scientific Research Institute for Atmospheric Air Protection, JSC
(SRI Atmosphere)

Introduction

The report outlines results of the NEASPEC project implementation by SRI Atmosphere in 2015-2016. The key tasks for the project were agreed at the joined Korea – Russia meeting conducted as a part of the Russian experts visit to Pusan National University (PNU) agenda in March 2015. These tasks cover the following:

1) Improvement of SRI Atmosphere's computational capacity (acquiring, installing and configuring a new server);
2) Preparation of emission data from the Russian sources of key pollutants (SO2, NOx and PM) for 2010 and capturing such emission data in the emission related fields of EDGAR database for 2008;
3) Deployment, launch and testing of WRF-CMAQ model on the new server at SRI Atmosphere to model quality of atmospheric air;
4) Estimation of average annual ground level concentrations as well as average complete deposition of sulfur and nitrogen oxides by means of WRF-CMAQ model system that is deployed on a multiprocessor server for meteorological conditions of 2010 based on the Russian emissions data as well as global emissions from the EDGAR database.

1. Improvement of SRI Atmosphere's computational capacity

In the course of the project the Russian experts have prepared a specification for the multiprocessor computer (server). Based on this specification the multiprocessor server was purchased. Required software was installed.

Key server specification elements along with the software installed are shown in Tables 1-3.

Table 1. Key specification elements of the multiprocessor complex (server)

Case	***Intel, P4304XXMUXX***
Motherboard	***Intel, S2600CW2S***
Processor	***Xenon E5-2697V3 (2 units)***
Hard drives	***HDD 3ТБ, Western Digital SE, WD3000F9YZ (4 units)***
Memory modules	***CT8G4RFS4213, Crucial 8GB DDR4 2133 MT/s (8 units)***

Table 2. Software for general purposes installed

Operational system SUSE Linux Enterprise Server, version 12	*CDO (Climate Data Operators) – library for operations with netCDF, GRIB -1,2 files of big size*
GNU Fortran (gfortran) 5.2.0 – Compiler Fortran 95 under GNU license	*GrADS 2.02 – graphical fields and data visualization system*

High performance computation cluster to perform mass-scale calculations Intel Parallel Studio XE 2016, including the following elements: *• Compilers Intel C++ and/or Fortran 95, the most cutting edge in the industry.* *• Mathematical library Intel Math Kernel to streamline performance.* *• Intel MPI Library 5.2.1 for Linux – Library for parallel calculations etc.*	*Support programs library:* *• zlib 1.2.8* *• hdf5 1.8.16* *• netCDF(C++) 4.4.0* *• netCDF(Fortran) 4.4.2* *• netCDF(C++ and Fortran) 3.6.1* *• MPICH-2* *• etc.*

Table 3. Software to facilitate correct operation of the WRF_3.6.1- CMAQ_4.7.1

WRF	***CMAQ***
• WPS 3.6.1 *• Jasper-1.900.1* *• netCDF-4.1.3* *• mpich-3.0.4* *• libpng-1.2.50* *• zlib-1.2.7*	*MPIC-3.6* *• cvc-1.12.10* *• netCDF-3.1* *• ioapi-3.1* *• senex-4.7.1* *• pario-4.7.1* *• and other*

2. The model description and testing

According to Pusan University specialists' recommendations, the WRF_3.6.1 - CMAQ_4.7.1 model was installed and launched on the multiprocessor server both in the basic and multiprocessor modes.

The WRF (Weather Research & Forecasting Model, ver. 3.6.1) model was combined with the transfer-photochemical atmospheric air quality CMAQ model (Model 3 Community Multi-scale Air Quality, ver. 4.7.1). Meteorological fields for 2010 were calculated via WRF model and further prepared by means of MCIP pre-processor in a corresponding format to be used in the CMAQ model.

2.1 Meteorological model

The WRF mesogrid meteorological model applied in this project represents a version of WRF-ARW (Advanced Research for Weather Forecasting) model, which in its turn represents an enhanced 5-th version of the mesogrid PennState/NCAR (MM5) model. The WRF model enables to calculate the key hydrodynamic variables in the sigma-system of axes with the upper limit ~ 100 GPa. The horizontal resolution of the model can be set within 1 to 150 km range.

Selection of parametrization schemes for key physical processes in the model was done according to recommendations given by Korean specialists during the Russian delegation's visit to PNU in October 2015. The above mentioned parameterization schemes are described in the 16th annual report on the joined (China, Republic of Korea and Japan) research results in the area of transboundary transfer of pollutants in the Northeast Asia (NIER, 2016).

Initial and boundary meteorological fields as of 2010 for modelling experiments with WRF were borrowed from the rda.ucar.edu (NCAR/UCAR) web-site in the form of GRIB2 files with 6-hour temporal resolution and spatial resolution of 1°x1° (1460 files altogether). These fields were further interpolated to the grid of the chosen model domain (Table 4, Figure 1) using a pre-processor of WRF model –WPS system.

The model domain was formed in such a way that it includes a main model area of the project (most part of China, Republic of Korea, and Japan) as well as the adjacent RF regions (Far East and Eastern Siberia). Characteristics of the chosen model domain are listed in the Table 4, and Figure 1 shows its geographical location.

Table 4. Model domain's characteristics

Projection	***Lamberta, conformal***
Central point	***120E and 45N***
Number of cells along the X axis	***120***
Number of cells along the У axis	***144***
1st standard latitude	***30N***
2nd standard latitude	***60N***
Cell size	***36000 meters***
22 *vertical sigma-levels*	**1.000, 0.995, 0.988, 0.976, 0.958, 0.933, 0.901, 0.862, 0.816, 0.763, 0.703, 0.636, 0.562, 0.481, 0.392, 0.302, 0.225, 0.165, 0.12, 0.080, 0.040 and 0.000**

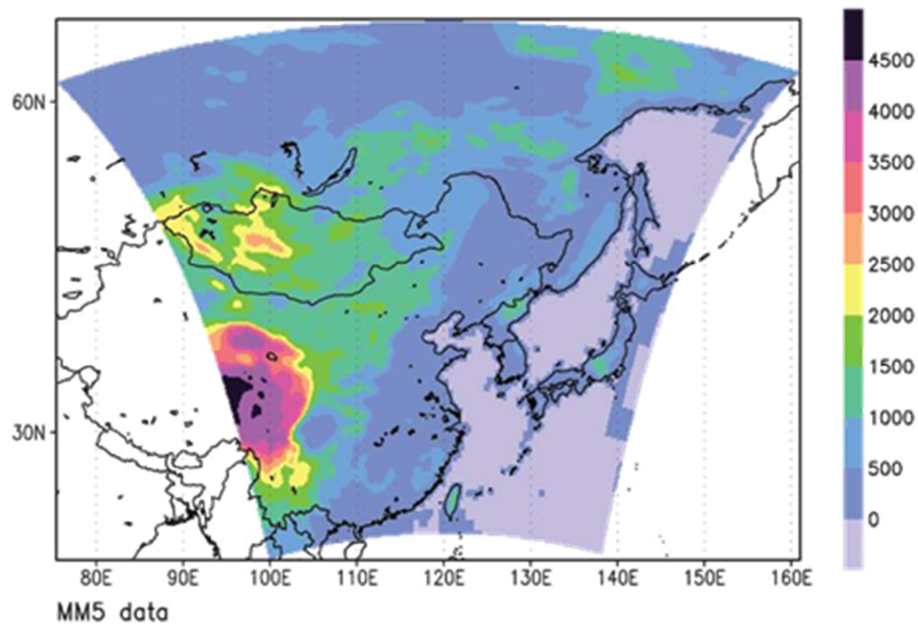

Figure. 1 Geographical location of the model domain (above sea level elevation, meters)

Input data on the land surface use, vegetation and soil types, land and marine areas distribution, surface relief and other similar information obtained from the U.S. data center USGS EROS for six horizontal special resolutions (from 30" to 1°) were also included in the model.

In order to validate correctness of installation and configuration of the WRF model on the acquired server the results of test calculation as per this model were compared with the similar calculation results as per MM5 model, applied at SRI Atmosphere and proved to be reliable.

For this end, via a special procedure (grib2to1) the files with initial and limit conditions for WRF model were converted from GRIB2 to GRIB1 format to enable further use of such files in MM5 model. Configuration of control files in MM5 model was automated and executed via editing of the single control file. By means of this file for MM5 model all the required parameters of the created domain (Figure 1) were defined. Further, meteorological fields in the given model domain were calculated for 2010 using the MM5 model.

Similar calculations were performed by means of the deployed WRF_3.6.1 model in the multiprocessor mode. At that, in order to set initial and limit conditions the GRIB2 meteorological fields were used that got prepared for launching similar calculations via MM5 model.

Key meteorological fields (Tem-2m, ground level pressure) calculated as per MM5 model for 2010 were compared with similar fields determined via WRF_3.6.1 model. Results of the comparison provided on the Figures 2-5 show a rather satisfactory reproducibility of the calculated fields enabling to conclude that the WRF model is installed and used correctly.

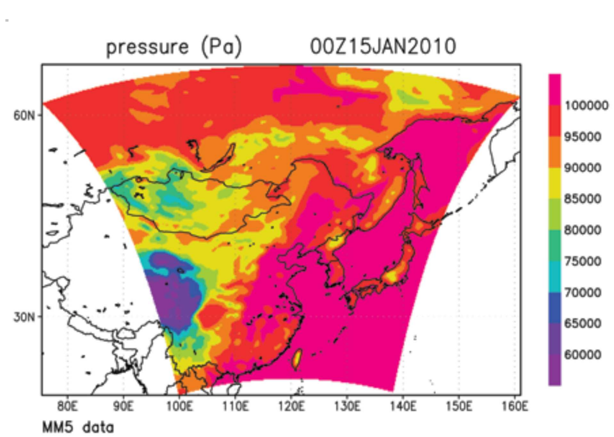

Figure 2. Ground level pressure (Pa) calculated with MM5 model, January 15, 2010 (00:00).

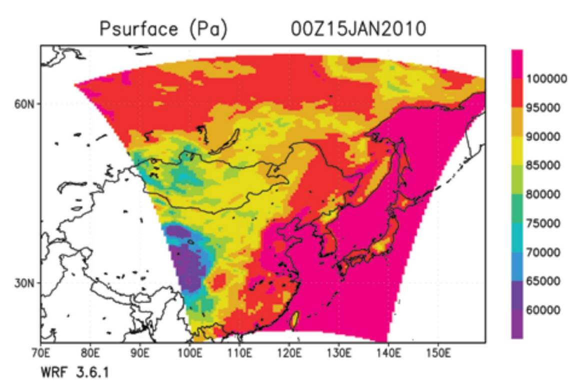

Figure 3. Ground level pressure (Pa) calculated with WRF model (3.6.1), January 15, 2010 (00:00).

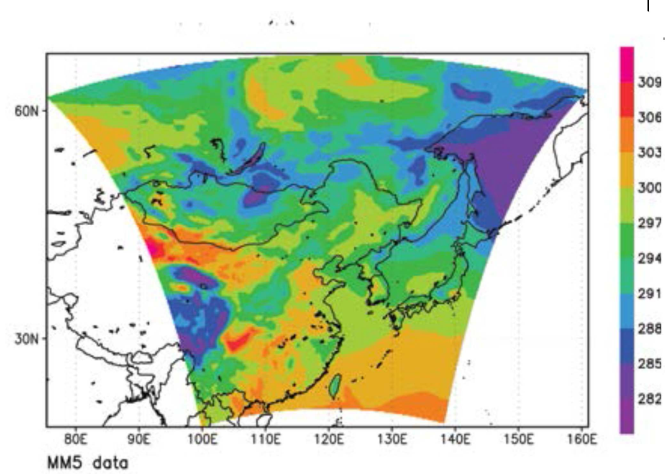

Figure 4 Temperature at 2m high from the surface (K) calculated as per MM5 model, January 15, 2010. (12:00).

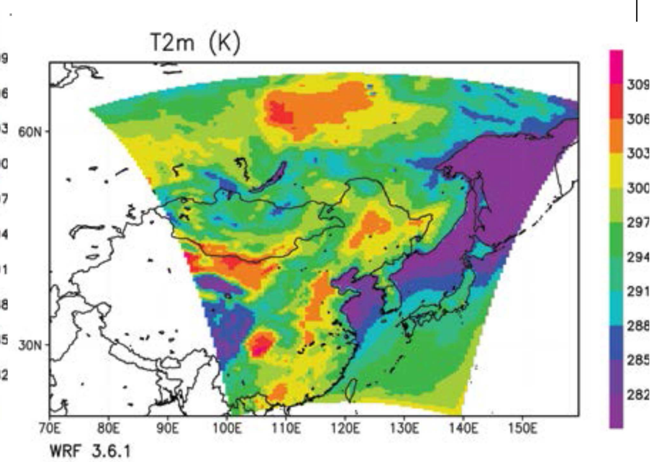

Figure 5 Temperature at 2m high from the surface (K) calculated as per WRF (3.6.1) model, January 15, 2010 (12:00).

2.2 Transport-photochemical atmospheric air quality model

Based on Korean experts' recommendations, the CMAQ 4.7.1. transport-photochemical atmospheric air quality model was installed on the acquired server. CB05cl mechanism was chosen as a photochemical scheme to estimate the content of gas atmospheric admixtures, and AERO 5 module was chosen for calculations of atmospheric aerosols concentrations.

The installed CMAQ 4.7.1 model was verified via a test recommended by the model developers. In this test the emission data and meteorological fields for the reference domain, as well as results of daily calculations of concentrations and fallout of pollutants based on such data via CMAQ 4.7.1 reference model are defined. The above test calculation was repeated using the CMAQ 4.7.1 model installed on the multiprocessor server. Comparison between the test calculation results against the reference one shows their agreement with high degree of accuracy (<0.01%).

The CMAQ-MCIP (Meteorology-Chemistry Interface Processor) model preprocessor converts the output meteorological fields of WRF to the required format for further use in the modelling experiments engaging the CMAQ model. At that, characteristics of the CMAQ model's model domain are similar to the corresponding characteristics of WRF model domain (Figure 1).
The CMAQ_4.7.1–WRF_3.6.1 model complex, installed on the new multiprocessor server was also tested by means of comparison of its results against the similar calculations performed using CMAQ_4.6.1–MM5_3 model complex that was applied by the SRI Atmosphere before. For this specific purpose the CMAQ 4.6.1 version was installed on the acquired multiprocessor server.

Then, two launches were prepared on the generated model domain, of which the first one – with CMAQ_4.7.1–WRF_3.6.1 model and the second – with CMAQ_4.6.1–MM5_3. Both launches baselined on the identical pollutants emission data from EDGAR database for 2008 (item 4 of this report).

Comparison of the results of the above model launches (CMAQ_4.6.1–MM5_3 and CMAQ_4.7.1–WRF_3.6.1) has shown a satisfactory compliance between the calculated concentrations and fallout of pollutants in 2010 on the generated model domain. The Figures 6 and 7 show the ground level SO_2 concentrations as of January 31, 2010 calculated using CMAQ_4.6.1 and CMAQ_4.7.1 models, correspondently illustrating comparison of the calculations. The Figures 8 and 9 show similar fields for calculated concentrations in case of ozone.

Analysis of the Figures enables to conclude that the calculated fields are qualitatively and quantitatively aligned and thereby once again verify that the CMAQ_4.7.1–WRF_3.6.1 model complex was installed and configured correctly.

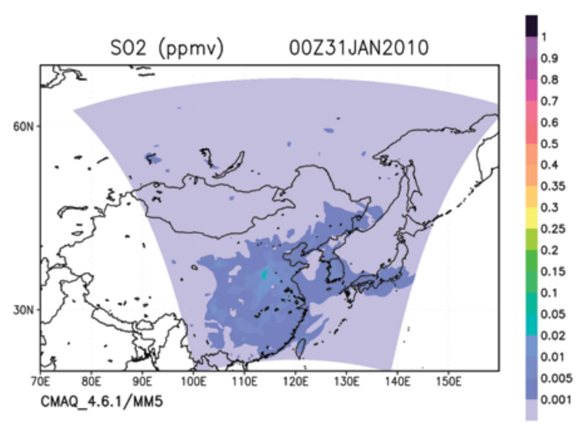

Figure 6. Ground level ratio of SO_2 mixture (ppmv) calculated using the CMAQ (4.6.1) - MM5, 31 January, 2010 (00:00).

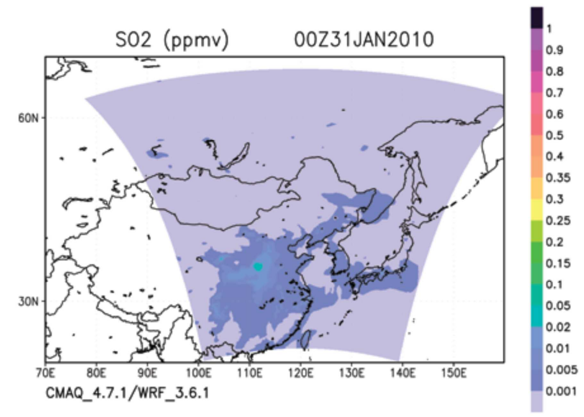

Figure 7. Ground level ratio of SO_2 mixture SO_2 (ppmv) calculated using the CMAQ (4.7.1) – WRF (3.6.1), 31 January 2010 (00:00).

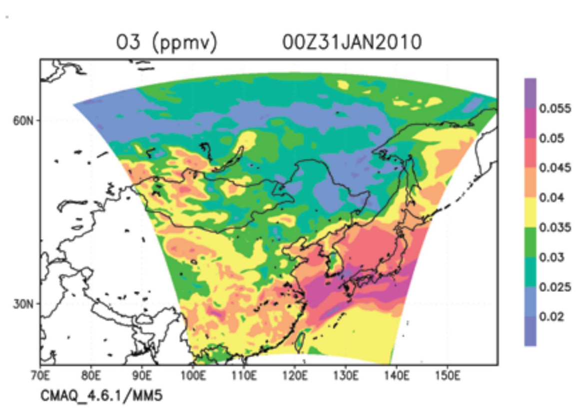

Figure 8. Ground level ratio of O_3 mixture (ppmv) calculated using the CMAQ (4.6.1) - MM5, January 31, 2010 (00:00).

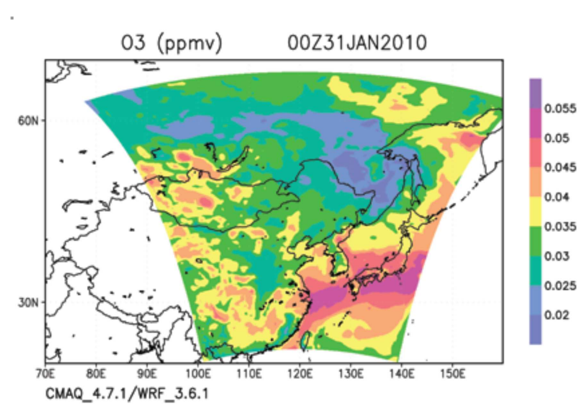

Figure 9. Ground level ratio of O_3 mixture (ppmv) calculated using the CMAQ (4.7.1) – WRF (3.6.1), January 31, 2010 (00:00).

2.2.1. Generation of emission data

The netCDF files containing emissions of major pollutants (SO_2, NOx, NMVOC, NH_3, CO and PM10) by main economic activity types for 2008 were downloaded from the EDGAR emission database web-site (**http://edgar.jrc.ec.europa.eu/overview.php?v=42**).

The files contain global geographical fields on annual emissions (kg*m-2s-1) with 0.1° x 0.1° horizontal resolution.

All downloaded data got interpolated to the grid of the generated model domain (Figure 1). For vertical distribution of emissions of pollutants the parametrization under the European program on monitoring and modeling of transboundary transfer (EMEP) was applied (Table 5). As per this parametrization the vertical emission distribution depends on a type of economic activity (fuel and energy complex, heavy industry, transportation and etc.).

Table 5 – Distribution of anthropogenic emissions from major source categories by vertical layers of the EMEP model (in %)

#	Source categories	Height of the emission layer (meters)					
		0-92	*92-184*	*184-324*	*324-522*	*522-781*	*781-1106*
1	Combustion in heat and power engineering	0	0	8	46	29	17
2	Non-commercial combustion plants	50	50				
3	Combustion in processing industry	0	4	19	41	30	6
4	Production processes	90	10				
5	Extraction and distribution of fossil fuel and geothermal energy	90	10				
6	Solvents and use of other products	100					
7	Road transport	100					
8	Other mobile sources and mechanical equipment	100					
9	Waste processing and disposal	10	15	40	35		
10	Agriculture	100					

Along with the emission data from EDGAR database the emissions (by types of economic activity) of major pollutants (nitrogen and sulfur oxides, and PM2.5) from the territory of the RF included in the model domain, for 2010 were prepared and presented in the required format.

Activities on collection and preparation of data on emissions of pollutants in question from the sources located in the regions of the RF for 2010 included in the estimated domain were performed step-by step.

As a part of step one, the Russian regions that either fully or partially included in the estimated domain were defined. Altogether, 17 Russian regions are included in the estimated domain, of which 11 constituents (Kemerovo region, Republic of Khakassia, Republic of Tuva, Irkutsk region, Republic of Buryatia, Trans-Baikal, Amur region, Khabarovsk territory, Jewish autonomous region, Primorye territory and Sakhalin region) – are included fully and 6 constituents (Yamal Nenets autonomous region, Khanty-Mansi autonomous region, Novosibirsk region, Krasnoyarsk territory, Republic of Sakha and Magadan region) – partially.

Further, in the ArcView GIS environment the boarders of the RF constituents were linked to the computational mesh cells via a splitting procedure of the Edit Tools module representing a set of scripts. As a result of this exercise the territory of the regions under investigation was presented as an aggregation of multiple cells.

Within the next step, calculation of the fractions occupied by territories of the constituents of the Russian Federation in the cells of the modeling domain was done. For this end, the area occupied by the territory of a specific RF constituent in a corresponding cell is divided by this cell's area.

Then, we collected and analyzed data on emissions of nitrogen oxide, sulfur oxide and PM in the territory of constituents of the RF that fall under the estimated domain for 2010 by industry sectors as well as large point sources-wise. Since currently in the Russian Federation PM2.5 emission volume estimation methodology is missing, emissions of this particular pollutant were estimated as a share of PM emissions (40%).

Data on emissions of the pollutants in question from heat and power facilities and large industrial enterprises were linked to the grid according to their geographical coordinates. Emissions from other economic activity types are evenly distributed across the cells of the grid, considering the fractions.

As a result of the performed activities the nitrogen oxide, sulfur oxide and PM2.5 emission values for 2010 were obtained from the sources in the constituents of the RF in each cell of the estimated domain, both – aggregated as well as by individual economic activity types.

Based on these data as well as emission data from EDGAR database for 2008 we prepared two sets of input emission files to make calculations as per CMAQ model. One set of data contains emissions of major pollutants taken from the EDGAR database for 2008. The second is similar to the first one apart from the territory of the RF for which emissions of SO2, NOx and PM2.5 from the EDGAR database were replaced with the corresponding Russian emission data for 2010.

Further we performed interpolation of both of the emission data sets to the chosen model domain along with conversion to the input format of the specifically developed code in FORTRAN and I/O API system of the CMAQ model.

Figures 10 and 11 show SO_2 emissions from EDGAR database for 2008 (tons per year from a cell of 36 km by 36 km dimension) as well as emissions prepared by the Russian experts for the RF territory for 2010 (tons per year from a cell of 36 km by 36 km dimension), correspondingly. Similar emission fields for nitrogen oxides are shown on the Figures 12 and 13.

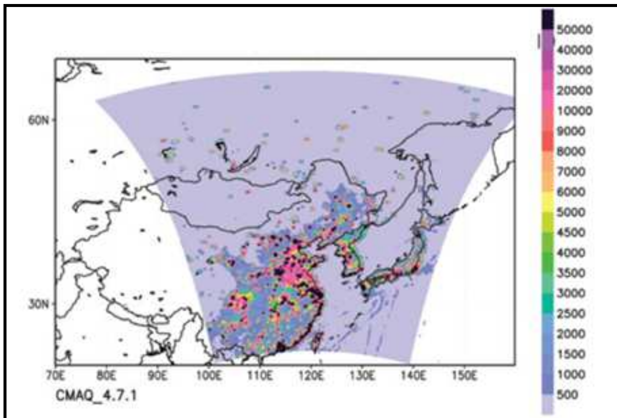

Figure 10. SO2 emissions (tons/year/cell) EDGAR, 2008

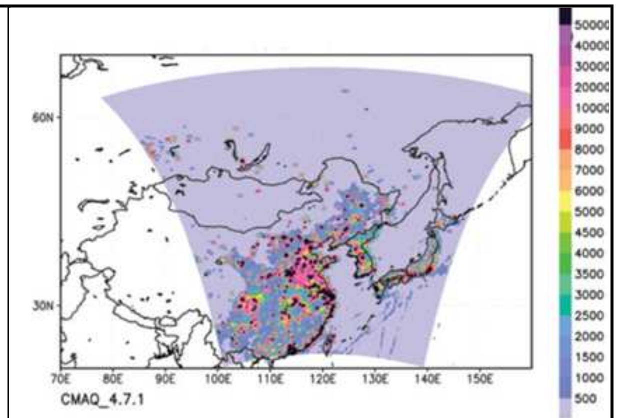

Figure 11. SO2 emissions (tons/year/cell), EDGAR(2008) + RF(2010)

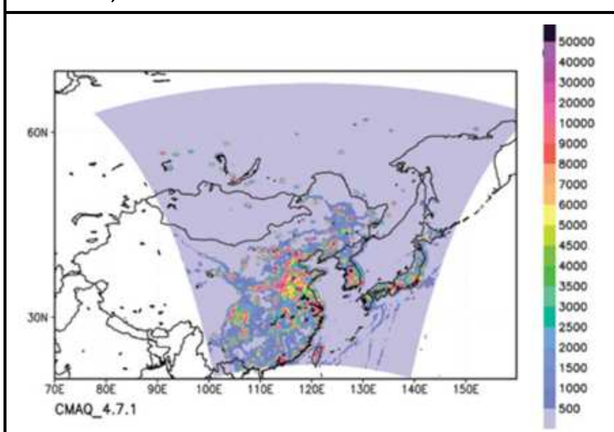

Figure 12. NOx emissions (tons/year/cell), EDGAR, 2008

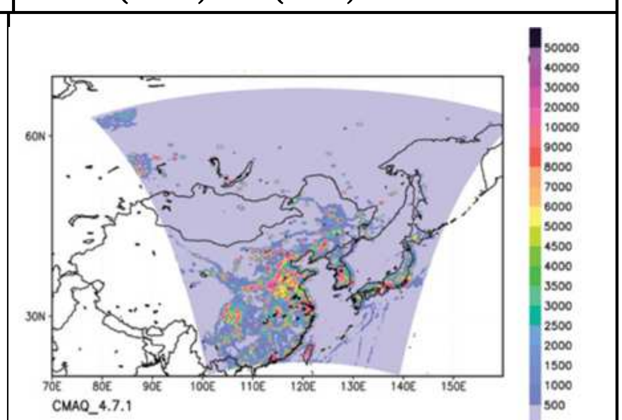

Figure 13. NOx emissions (tons/year/cell), EDGAR(2008) + RF(2010)

2.2.2. Atmospheric transfer of pollutants modeling results using CMAQ_4.7.1- WRF_3.6.1 model system

The CMAQ_4.7.1-WRF_3.6.1 model system deployed on the new multiprocessor server (section 1) and tested (section 2) was used for calculations of average annual ground level concentrations (Figures 14-17) and full annual depositions (Figures 18 and 19) of major pollutants for the chosen model domain (Figure 1). At that, we used meteorological fields as of 2010 calculated using the WRF_3.6.1 model as well as emission data from EDGAR database as of 2008 combined with the emission data from RF territory as of 2010 prepared by SRI Atmosphere as a part of this project (1-st modelling experiment). Besides, we did the annual calculation that is fully identical to the one described above, however only using emissions from EDGAR for 2008, without consideration of the SRI Atmosphere's emission data (2-nd modelling experiment).

Figures 14 and 15 show geographical distributions of average ground level concentrations of sulfur oxide calculated in the first and second modelling experiments with the CMAQ_4.7.1-WRF_3.6.1 model system described above. The Figures 16 and 17 show geographical distribution of calculated ground level concentrations of NOx.

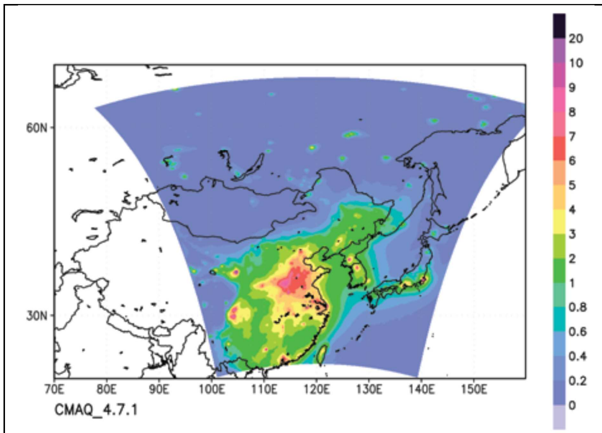

Figure 14. Ground level average annual ratio of SO_2 (ppbv) calculated using the CMAQ_4.7.1 - WRF_3.6.1, 2010, EDGAR emissions

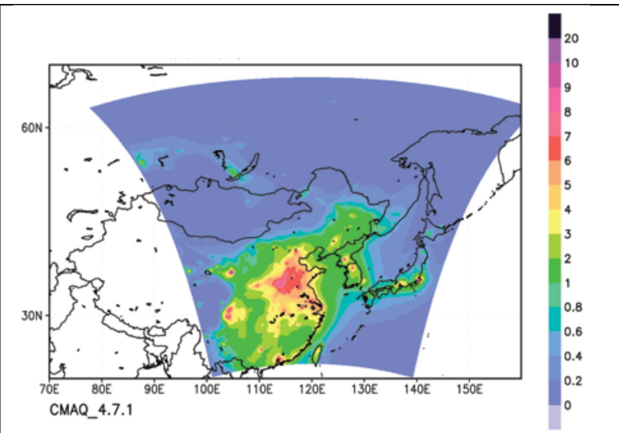

Figure 15. Ground level average annual ratio of SO_2 (ppbv) calculated using the CMAQ_4.7.1 – WRF_3.6.1, 2010, EDGAR+RF .

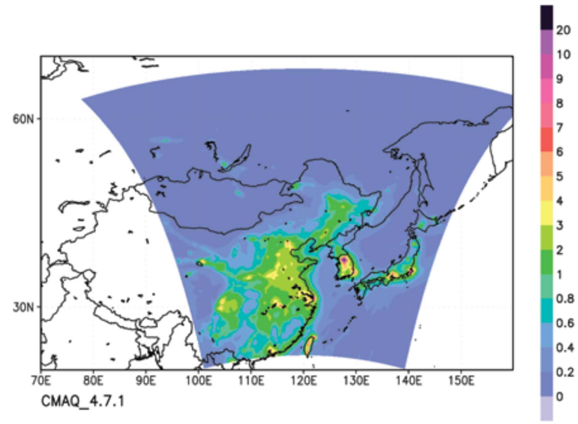

Figure 16. Ground level average annual ratio of NO_X (ppbv) calculated using the CMAQ_4.7.1 – WRF_3.6.1, 2010, EDGAR emissions

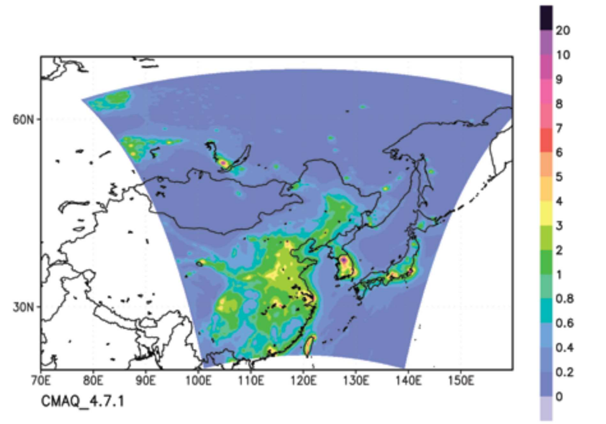

Figure 17. Ground level average annual ratio of NO_X (ppbv) calculated using the CMAQ_4.7.1 – WRF_3.6.1, 2010, EDGAR+RF emissions

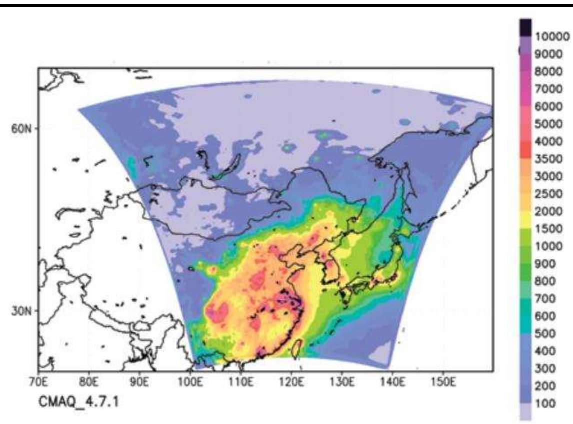

Figure 18 Annual fallouts of oxidized sulfur (mgS/m2) calculated by CMAQ_4.7.1 – WRF_3.6.1 model, 2010 EDGAR emissions

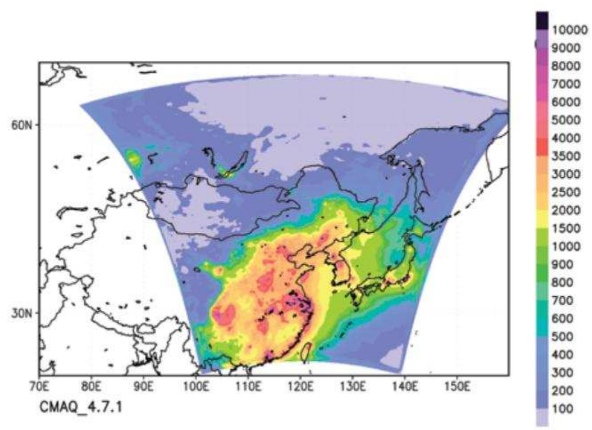

Figure 19 Annual fallouts of oxidized sulfur (mgS/m2) calculated by CMAQ_4.7.1 – WRF_3.6.1 model, 2010, EDGAR+RF emissions

The Figures 14 and 15 show that geographical distribution of ground level SO_2 concentrations correspond to spatial distribution of its emissions. The local peaks of the ground level concentrations are observed at the North-East of China as well as at the industrial areas of Japan and South Korea. Comparison between the Figures 14 and 15 enables to conclude that input of emission data prepared by SRI Atmosphere to EDGAR database, substantially changes ground level concentrations of SO_2 in the RF territory within the chosen model domain. In the vicinity of Baikal Lake, in the areas neighboring with Kazakhstan the ground level concentrations of SO_2 from the 1-st experiment significantly exceed concentrations attributed to the 2-nd experiment (where only EDGAR emission data is used). In the territory of East Siberia and Far East the opposite situation is encountered such as involvement of SRI Atmosphere's emission data results in a reduction of the ground level SO_2 concentrations to a certain degree.

Analysis of Figures 16 and 17 enables to come to the same conclusions with regards to geographical distribution of NO_X. The key distinction is related to the fact that use of emission data prepared by the Russian specialists in calculations results in a significant increase of ground level concentrations across the entire RF territory, included in the chosen domain.

Inclusion of SO_2 as well as NO_X emission data provided by SRI Atmosphere to the inputs for CMAQ-WRF calculations neither significantly impacts ground level concentrations, nor depositions of sulfur and nitrogen oxides in China, Republic of Korea and Japan.

Conclusions

The key tasks of the project were discussed and formulated during the Korea-Russia joined meeting as a part of the Russian scientists visit to Pusan University in March 2015.

All the tasks given in the beginning of the project are fully accomplished. Through the project the cutting-edge multiprocessor server was acquired and installed at SRI Atmosphere. All required software, including the CMAQ_4.7.1-WRF_3.6.1 was installed on the server. This model system was tested both by means of the test proposed by the model developers, as well as via comparison of the fields calculated using it with the similar results obtained via the CMAQ_4.6.1-MM5_3 model system that is already well tested by SRI Atmosphere.

Finally, the CMAQ_4.7.1-WRF_3.6.1 model system was used to calculate ground level concentrations of sulfur and nitrogen oxides on the selected model domain. At that, the emission data prepared by the Russian specialists for the territory of the RF along with the emission fields from EDGAR database were utilized as input emission data.

The results of model calculations lead to the following conclusions:

1. Spatial distribution of the ground level concentrations of SO2 and NOx is closely related to the corresponding geographical emission distribution;
2. Max concentration values correspond to the main industrial areas in China, Japan and Republic of Korea;

3. Sources of pollutants in the territory of the RF do not significantly contribute to the state of pollution of the air basin in China, Republic of Korea and Japan areas;
4. If instead of EDGAR data base emission data the emissions prepared by the Russian specialists are used the estimated emissions of pollutants in the territory of the RF within the model domain will increase significantly.

The CMAQ_4.7.1–WRF_3.6.1 model recommended by the Korean side for the deployment has successfully passed testing on the multiprocessor server at SRI Atmosphere and became reputable due to high level of calculation quality and performance. The decision was made to continue using it in the research projects going forward.

List of references

1. NIER-GP2016-032: The 16th year's Joint Research on Long-range Transboundary Air Pollutants in Northeast Asia, March 2016, ISBN 978- 89-6558-341-7.